

LEE-YANG ZEROS FOR SUBSTITUTIONAL SYSTEMS

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ABSTRACT

Qualitative and quantitative information about critical phenomena is provided by the distribution of zeros of the partition function in the complex plane. We apply this idea to Ising models on non-periodic systems based on substitution. In 1D we consider the Thue-Morse chain and show that the magnetic field zeros are filling a Cantor subset of the unit circle, the gaps being related to a general gap labeling theorem. In 2D we study the temperature zeros of the Ising model on the Ammann-Beenker tiling. The use of corner transfer matrices allows an efficient calculation of the partition function for rather large patches which results in a reasonable estimate of the critical temperature.

1. Introduction

In 1952, Lee and Yang presented a new approach to questions like the existence and location of critical points⁹. They proposed to treat the field or fugacity as complex variables and to investigate the zeros of the partition function in the complex plane. Later, also the zeros in the complex temperature plane were studied, they also yield information about phase boundaries as well as critical exponents. For regular isotropic lattices, these zeros typically lie on simple curves (though they can fill 2D regions in anisotropic cases). But for hierarchical graphs, they generally form fractal structures⁶. Non-periodic graphs with inflation symmetry may be regarded as a link between the extensively studied regular and hierarchical models. So one expects them to combine aspects of both classes. This is why we study the Ising model on certain aperiodic graphs based on substitution rules.

For the classical 1D Ising model on the Thue-Morse chain we will show the appearance of fractal structures in the patterns of *magnetic field zeros* – a consequence of non-commuting transfer matrices for this special aperiodic order. In 2D, however, these zeros did not show any interesting structures³. Therefore, we present the *temperature zeros* of an Ising model on a quasiperiodic graph, namely the so-called Ammann-Beenker tiling. Its symmetry and the technique of corner transfer matrices allow an efficient numerical treatment of quite large patches.

2. Ising Model on the Thue-Morse Chain

Let us start with the discussion of a 1D chain of N Ising spins $\sigma_j \in \{\pm 1\}$ with periodic boundary conditions ($\sigma_{N+1} = \sigma_1$). The energy of a configuration σ reads:

$$E(\sigma) = - \sum_{j=1}^N (J_{j,j+1} \sigma_j \sigma_{j+1} + H_j \sigma_j) . \quad (1)$$

Here, we consider a system with uniform magnetic field $H_j = H$ where the couplings $J_{j,j+1}$ take only two different values J_a, J_b according to the two letters of the Thue-Morse chain.

The latter is obtained through the substitution rule

$$S : \begin{array}{l} a \rightarrow ab \\ b \rightarrow ba \end{array} \quad (2)$$

where we consider the successive periodic systems obtained from the words a , ab , $abba$, $abbabaab$ and so on by cyclic closure. The partition function may be written as the trace of 2×2 transfer matrices⁴. Introducing the notation $z_{a,b} = \exp(2\beta J_{a,b})$ and $w = \exp(2\beta H)$, where β is the inverse temperature, the two elementary transfer matrices T_a and T_b read:

$$T_{a,b} = (wz_{a,b})^{-1/2} \begin{pmatrix} wz_{a,b} & w^{1/2} \\ w^{1/2} & z_{a,b} \end{pmatrix}. \quad (3)$$

The recursion relation for the chain is the same as that for the transfer matrices, and so the essential part of the partition function is evidently a polynomial^{2,3} in the three variables z_a , z_b and w .

In what follows, we restrict ourselves to the ferromagnetic regime (i.e. $z_a, z_b \geq 1$), focusing on the magnetic field zeros for fixed positive temperature. Due to the quite general Lee-Yang theorem⁸ the magnetic field zeros are restricted to the unit circle. For a periodic chain the zeros can be calculated analytically¹⁰, where they fill a connected part of the unit circle densely in the thermodynamic limit. The only gap is near the positive real axis, due to the fact that there is no phase transition for finite temperature in 1D. In Fig. 1 we show

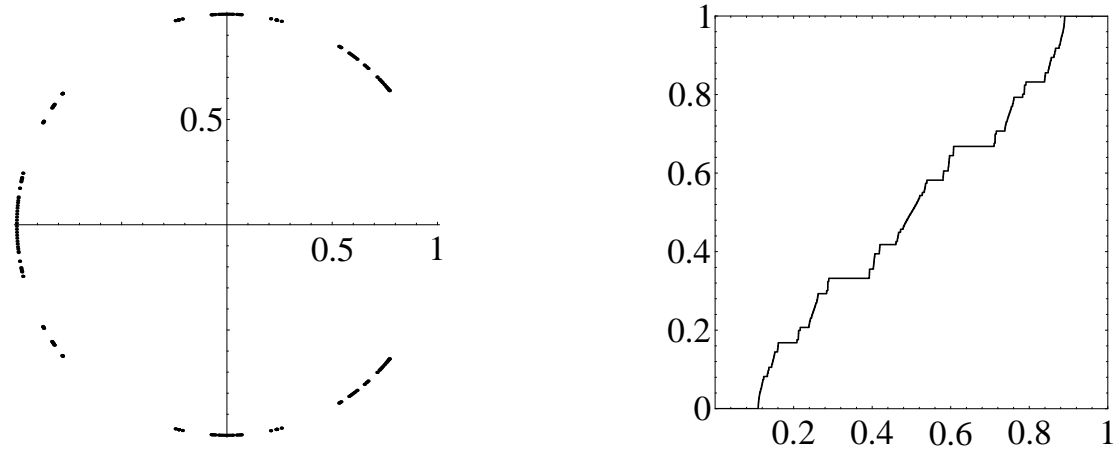


Fig. 1. Magnetic field zeros and their integrated density on the unit circle.

the magnetic field zeros of the Thue-Morse chain in the w -plane in the ferromagnetic case $z_a = 3/2$, $z_b = 100$ for the periodic approximant of length $2^8 = 256$. As expected, the gap around the real axis near the point $w = 1$ is still present. But there is, in fact, an infinite hierarchy of gaps, each with the well-known Lee-Yang edge singularity. It is an interesting property that these gaps (through the definition of a discrete step function along the unit circle) may be related to the gap labeling in the electronic spectrum of the Thue-Morse chain, for details see Refs. 2 and 5.

3. Ising Model on the Ammann-Beenker Tiling

Exact results for 2D quasiperiodic models are rather rare and generally restricted to very special cases. Even for systems with an inflation symmetry no exact renormalization is known for electronic systems or Ising models. So, we apply a combination of an exact

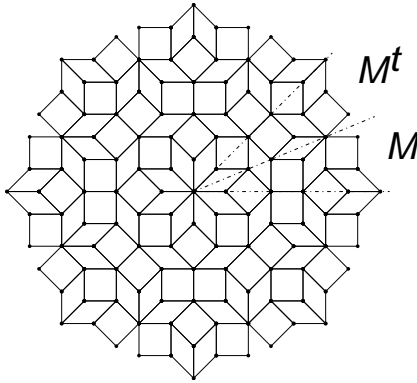


Fig. 2. Octagonal patch of the Ammann-Beenker tiling.

calculation of a finite partition function followed by an investigation of the complex zeros as an approach to the thermodynamic limit.

For our 2D quasiperiodic Ising model, we have chosen the Ammann-Beenker tiling¹. It has only one kind of edges, which suggests a simple choice of equal couplings along all bonds. But it is even more important that the octagonal symmetry allows the application of corner transfer matrices⁴. It may be built repeating the indicated small sector 16 times. The corresponding (rectangular) corner transfer matrix \mathbf{M} is easy to calculate. Consequently the partition function $Z(w, z)$ is simply given by:

$$Z(w, z) = \text{tr} \left((\mathbf{M}^t \mathbf{M})^8 \right). \quad (4)$$

This simple structure allows the exact calculation of the partition function for large patches using algebraic manipulation packages. So our calculations were limited by the degree of the resulting polynomial partition function, as the numerical calculation of polynomial roots quickly becomes really involved.

In contrast to 1D, the magnetic field (w) zeros do not seem to contain any relevant new information: their angular distribution looks astonishingly regular in comparison to the 1D case, and no gap structure is visible. So, we concentrate on the temperature (z) zeros here and restrict ourselves to the case of zero magnetic field. In Fig. 3, the temperature zeros

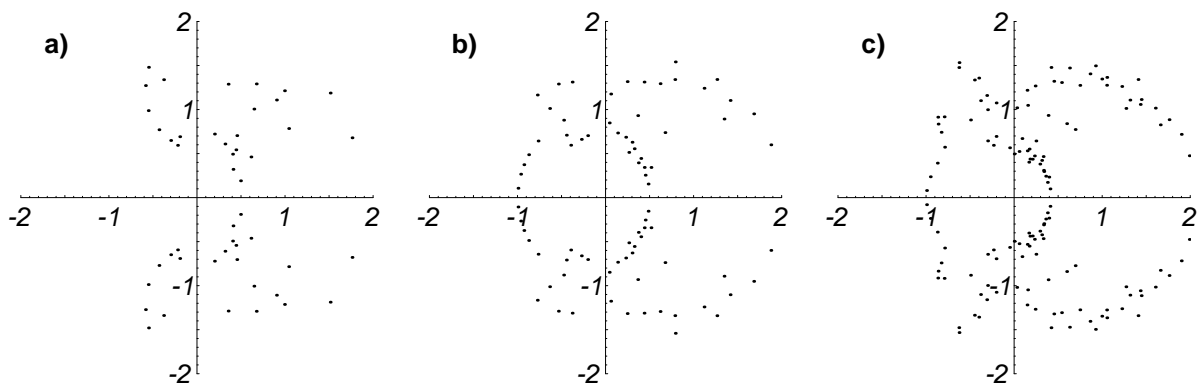


Fig. 3. Partition function zeros in the complex temperature plane.

are shown for a growing sequence of patches with fixed boundary conditions, with Fig. 3c) corresponding to the patch shown in Fig. 2. In principle the zeros do not appear to lie on simple curves. But those near the real axis directly contain information about the critical point and indirectly even about critical exponents (for which one would need to know the

dependence of the zeros on the magnetic field). Fig. 3 shows alignments of zeros ($Re(z) > 1$) converging towards two points of the real axis. The numerical values of the zeros closest to the critical ferromagnetic as well as antiferromagnetic couplings are given in Table 1. In the ferromagnetic case they are in very good agreement with the specific heat and center spin magnetization also obtained by numerical calculations. In comparison to the square lattice (where the critical coupling is $z_c = 1 + \sqrt{2}$), the local coordination looks a bit higher (though its average is strictly 4), and the critical coupling shows this by a slight decrease in agreement with other results⁷. As our graph is bipartite, the critical antiferromagnetic coupling is just the reciprocal of the ferromagnetic one. Due to the fixed boundary conditions, which are not appropriate for the antiferromagnetic case, we expect our numerical values to show large finite-size effects there.

Table 1. Zeros of the partition function closest to the real axes.

	a)	b)	c)
Ferromagnetic:	$1.7608 \pm 0.6795i$	$1.8772 \pm 0.5993i$	$1.9895 \pm 0.4752i$
Antiferromagnetic:	$0.4944 \pm 0.1906i$	$0.4834 \pm 0.1543i$	$0.4075 \pm 0.0988i$

4. Conclusion

Our 1D calculations showed the fractal structure of the magnetic field zeros for 1D non-periodic Ising models, while this structure seems to be absent in 2D. This and the relation to a gap labeling is quite similar to the electronic and vibrational spectra. For 2D Ising like systems the investigation of partition function zeros yields valuable information about the critical point of models on quasiperiodic graphs. Their distribution is rather more complicated than for regular periodic graphs but the location of the ferromagnetic phase transition clearly shows up where the zeros "pinch" the real axis.

5. References

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